

T-4
Atomic & Optical Theory

Fermion Molecular Dynamics

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Classical dynamics, often called “molecular dynamics” when applied to atoms and molecules, is usually much easier than solving the many-body Schrödinger equation. Whereas quantum mechanics involves fields and wave functions, and hence an infinite number of degrees of freedom, classical mechanics involves $6N$ degrees of freedom for an N -body system. In particular, correlation and rearrangement are simple in classical dynamics. Fermion molecular dynamics (FMD) is a quasiclassical method for treating quantum-mechanical systems using classical equations of motion with model potentials to constrain the motion to satisfy the Heisenberg uncertainty and the Pauli exclusion principles.

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molecules, the effective Hamiltonian automatically provides an atomic shell structure.

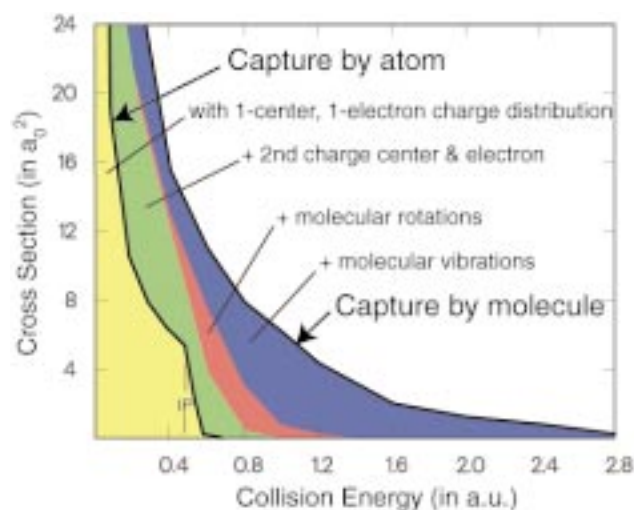


Figure 1: Cross sections as a function of collision energy for antiproton capture by the hydrogen atom and molecule, with the approximate contributions due to target two-center structure, rotations, and vibrations. The atomic ionization potential is marked by IP.

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behavior can be enforced by the constraining inequality, $r_{ij}p_{ij} \geq \xi_p \hbar$, where r_{ij} and p_{ij} are the relative position and momentum of electrons i and j . The quantum connection comes from the (reduced) Planck's constant \hbar , and ξ_p is a dimensionless parameter of order unity. Similarly, the Heisenberg principle demands that a particle cannot be localized in position and momentum; e.g., all electrons satisfy $r_i p_i \geq \xi_H \hbar$ with respect to a nuclear center. The model goes to the classical limit for ξ_p and ξ_H set to zero. In practice, the inequalities are replaced by momentum-dependent pseudopotentials, V_p and V_H , which simulate and smooth these constraints. V_p and V_H are added to the usual Hamiltonian, and the system evolves in time according to Hamilton's classical equations of motion. The purpose of the constraining potentials is simply to avoid quantum mechanically forbidden regions of phase space. In addition to stabilizing all atoms and many

It is for dynamics, as its name suggests, that the FMD method manifests its power. The method has been used to tackle some problems for which no practical quantum-mechanical methods are currently available. The quasiclassical treatment can also provide guidance to development of effective new quantum-mechanical methods by illuminating the physical features that need to be treated. The FMD method has been applied to atomic and molecular structure, ion-atom collisions, stopping powers, multiple ionization of atoms in strong laser fields, and, discussed below, formation of exotic atoms.

In an exotic atom, a negative muon μ^- (207 times as massive as an electron), a negative pion π^- (273 times as

massive as an electron), or an antiproton \bar{p} is bound to a normal nucleus. The most studied, experimentally and theoretically, and fundamental of these atoms is antiprotonic hydrogen, $\bar{p}p$. Already in this simplest case, there is an experimental-theoretical disconnect. All the experiments have been done with a molecular H_2 target, while past theoretical subjects have been an atomic H target or frozen molecule (a new experimental facility is now under construction that will also be able to use atomic hydrogen targets).

Both the FMD and time-dependent quantum-mechanical methods have been applied to muon capture by the H atom and yield results in good agreement. However, for the H_2 molecule the usual implementation of time-dependent quantum mechanics via the Hartree-Fock method does not suffice since the hydrogen molecule does not dissociate correctly in that approximation. The FMD method treats all the molecular degrees of freedom as well as the particle rearrangement, electronic continuum, and correlation that are also important in the reaction.

The expectation that the H_2 molecular target would be similar to the H atomic target turned out to be stunningly wrong. The \bar{p} capture cross sections for the atom and the molecule (see Figure 1) show that capture by the atom cuts off sharply above the ionization threshold but capture by the molecule extends to much higher energies. The effects due to the two-center structure, rotational motions, and vibrational motions are all taken into account by the FMD calculation, but it is mainly the vibrational degree of freedom, as shown in the figure, that enables the molecule to capture antiprotons at the higher energies. The mechanism seen in most capture trajectories (see Figure 2) is that one electron is ionized upon close approach of the \bar{p} , leaving behind an unstable $pp\bar{p}e$ complex (Figure 2c). At the higher energies this first ionization is usually prompt, but at low energies a five-body precursor complex often survives for several vibrational periods (Figure 2b). The $pp\bar{p}e$ complex then usually dissociates into $\bar{p}p + \text{H}$ after the first-ejected electron is far removed (Figure 2d).

In similar calculations, we have also explained results of a 1996 experiment on antiprotons in H_2 vs. D_2 that revealed an unexpected isotope effect on stopping, as well as an old series (1969 to 1990) of experiments on pion capture in HD vs. $\text{H}_2 + \text{D}_2$ mixtures, which had previously been subject to a misinterpretation yielding an incorrect pion transfer probability.

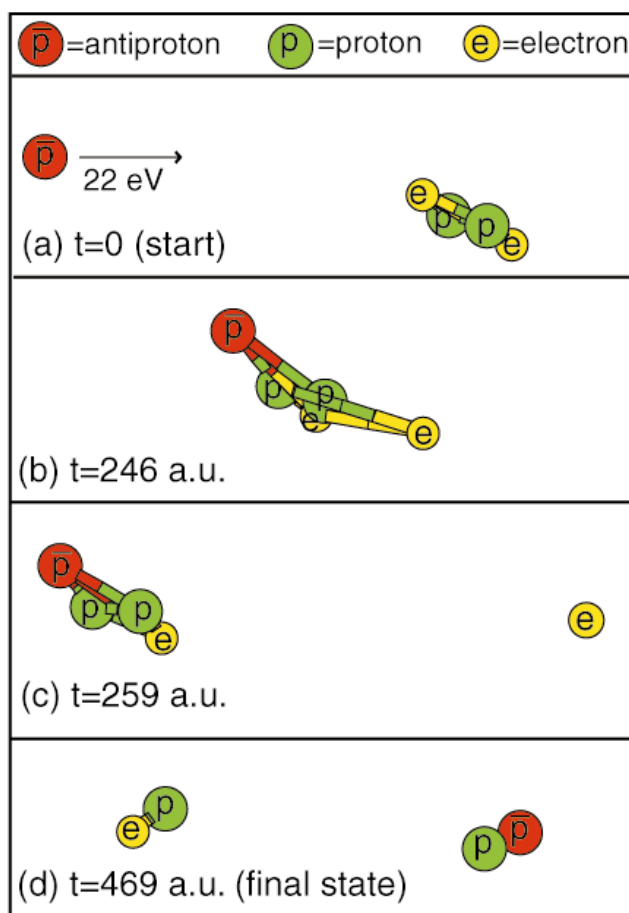


Figure 2: Snapshots of a typical trajectory at four different times (t) in which an antiproton is captured by a hydrogen molecule.